

Walkup MS Report



Data File mlo416_Pos_LoopInjection_MS_fragile2_01317.d
Sample Type Sample
Instrument Name 6545 QTof
Acq Method Pos_LoopInjection_MS_fragile2.m
IRM Calibration Status Success
Comment

Sample Name mlo416
Position P1-A1
User Name Maria Odyniec
Acquired Time 1/8/2019 10:54:08 AM
DA Method Pos_LoopInjection_MS_fragile2.m

Sample Group
Walkup Sample Description
Formula C46H43BCIN3O7
Stream Name LC 1

Info.
Walkup Method Pos_LoopInjection_MS_fragile
Walkup Method Description Lower fragmentor and Rf voltages in positive mode loop injection for fragile ions
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

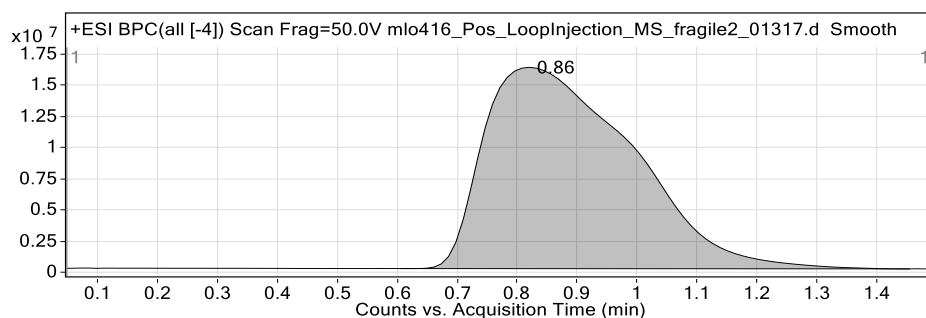


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.86	279426562	100.00	100.00	156.1510	0.300

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C46 H43 B Cl N3 O7	1.02	796.2949	794.2905	794.2919	-1.78	99.21

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

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Compound specific information

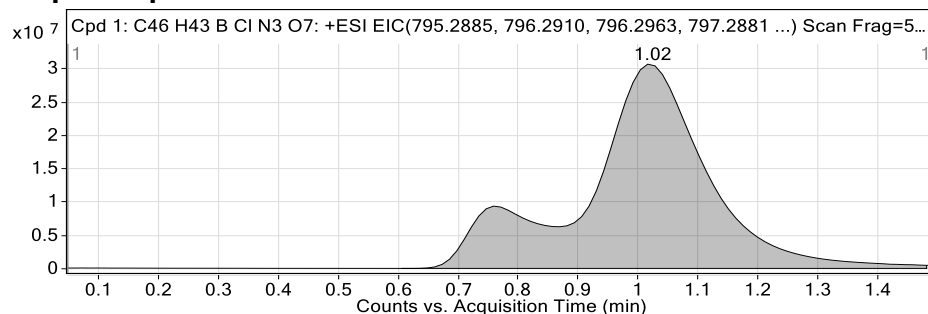


Figure: Extracted ion chromatogram (EIC) of compound.

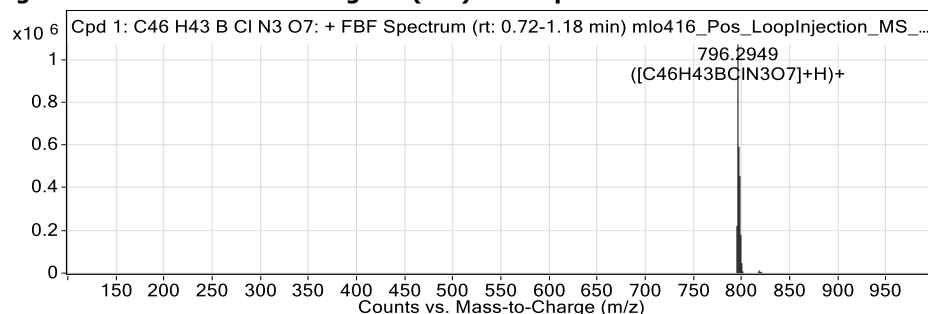


Figure: Full range view of Compound spectra and potential adducts.

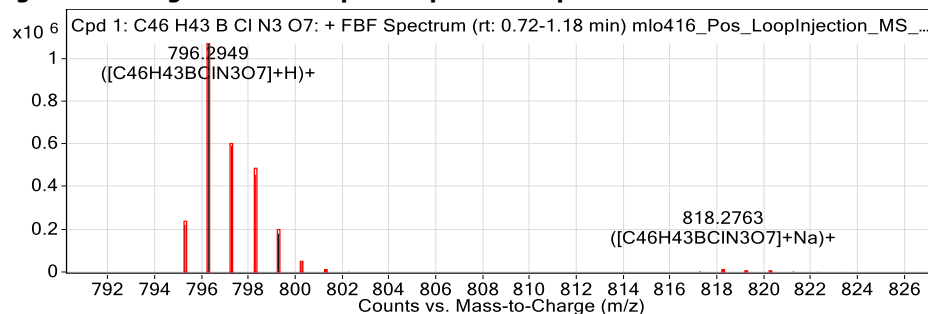


Figure: Zoomed Compound spectra view

(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
795.2977	1	221401.2	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
796.2949	1	1069636.9	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
797.2974	1	590657.8	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
798.2948	1	454672.3	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
799.2961	1	178867.6	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
800.2980	1	46548.9	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
801.3008	1	8610.6	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+H)+
817.2796	1	2913.9	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+Na)+
818.2763	1	12477.3	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+Na)+
819.2788	1	7081.0	C ₄₆ H ₄₃ BCIN ₃ O ₇	(M+Na)+

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